Appendix F
Ecotoxicity Profiles for Munitions Compounds

The document *Organic Explosives and Related Compounds: Environmental and Health Considerations* (Technical Report 8901, U.S. Army Medical Bioengineering Research and Development Lab, 1989) presents extensive discussion on the synthesis and production and use of organic explosives and related compounds. This document also discusses properties, behavior, and environmental fate of organic explosives and related compounds, and includes toxicity profiles of some compounds. Tables 1, 6, and 7, in Appendix F1, are from this document. This document is referenced by several more recent documents which provide toxicity information about specific compounds.

A more thorough toxicity assessment of several compounds is presented in a U.S. Army Environmental Health Agency (USAEHA) document. Sections presenting toxicity profiles for 2,4,6-TNT (Section 3.1.1) and DNT (Section 3.1.2) in ecological receptors are reproduced in this appendix as Appendixes F2 and F3.

The USAEPA prepares ecotoxicity profiles for organic explosives as well. Copies of these profiles for 2,4,6-Trinitrotoluene, Nitrobenzene, 1,2-Dinitrobenzene, p-Dinitrobenzene, 1,3,5-Trinitrobenzene, 2,6-Dinitrotoluene, 1,3-Dinitrobenzene, and Benzenamine are included in Appendix F4.

Other Sources

Another source of information on several compounds, including general toxicity characteristics, for the metals As, Cd, Cr, Pb, and Hg; the explosives, 1,3-Dinitrobenzene, 2,4-Dinitrotoluene (2,4-DNT), 2,6-Dinitrotoluene (2,6-DNT), HMX, RDX, Tetryl, 1,3,5-Trinitrobenzene, 2,3,6-Trinitrotoluene (2,4,6-TNT); and the pesticides DDD, DDE, and DDT are presented in a USAEHA Joliet document.

Other sources of toxicity information regarding TNT are:

- Palazzo, A.J., and D.C. Leggett, 1986. Effect and disposition of TNT in a terrestrial plant and validation on analytical methods. USCOE, CRREL Report 86-15.

- Caltado, D.A., S.D. Harvey, R.J. Fellows, R.M. Bean, and B.D. McVeety, 1989. Environmental Fate and Behavior of TNT. An Evaluation of the Environmental Fate and Behavior of Munitions Material (TNT, RDX) in Soil and Plan Systems, Pacific Northwest Laboratory, Project Order No. 88PP8853.

Another source of toxicity information regarding RDX is:

. Cataldo, D.A., S.D. Harvey, and R.J. Fellows, 1989. Environmental Fate and Behavior or RDX. An Evaluation of Environmental Fate and Behavior of Munitions Material (TNT, RDX) in Soil and Plant Systems, Pacific Northwest Laboratory, Project Order No. 88PP8853.

Appendix F1
Tables

Source: Burrows, E. P., D.H. Rosenblatt, W.R. Mitchell, and D.L. Parmer, 1989. Organic Explosives and Related Compounds: Environmental and Health Considerations. Technical Report 8901, U.S. Army Medical Bioengineering Research and Development Lab.

* Figure 1 and the references cited are not included in this excerpt.

INTRODUCTION

Explosives and propellants have important military applications; the former are also widely used in mining and construction. Their manufacture represents a sizable segment of the chemical industry [I]. In the course of production, handling, loading of military or civilian devices, and ultimate dispersal or disposal, explosives and propellants *are* released to the environment. There they are disseminated by natural processes and partially converted to secondary products. This report deals only with the more important organic explosives and propellants, and the focus is primarily on physicochemical properties and behavior, environmental fate, toxicity to human beings and wildlife, and environmental criteria; a comprehensive review that emphasizes manufacturing processes, formulations and uses is available [2]. While reasonable attempts have been made to assemble all pertinent material, some sources will doubtless have been missed. In addition to such omissions, there are extensive gaps in our knowledge, especially of environmental fate and chronic toxicity. Table 1 is a summary of the compounds to be covered and the abbreviated names for them that will be used throughout the report.

Table 1. Listing of Explosives, Propellants, and Derived Substances

Compound[a]	Abbreviation
Trinitrotoluene[b]	TNT
Dinitrotoluene[c]	DNT
1,3,5-Trinitrobenzene	TNB
1,3-Dinitrobenzene	DNB
Hexahydro-1,3,5-trinitro-1,3,5-triazine	RDX
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	HMX
1-Acetylhexahydro-3,5-dinitro-1,3,5-triazine	TAX
1-Acetyloctahydro-3,5,7-trinitro-1,3,5,7-tetrazocine	SEX
N,2,4,6-Tetranitro-N-methylaniline	Tetryl
Ammonium picrate/Picric acid	AP/PA
Pentaerythritol tetranitrate	PETN
Nitroglycerin (glyceryl trinitrate)	NG
Nitroguanidine	NQ
Ethylene glycol dinitrate	EGDN
Diethylene glycol dinitrate	DEGDN
Propylene glycol dinitrate	PGDN

a. Structures are presented in Figure 1.
b. Where TNT is used, the 2,4,6-isomer (formerly known as u-TNT) is denoted; other isomers are specifically designated, e.g. 2.3.4-TNT.
c. Where DNT is used, the 2,4-isomer is denoted, possibly with minor amounts of other. isomers -- especially the 2,6-isomer; other isomers are specifically designated, e.g. 2,3-DNT.

Table 6. Acute Toxicities of Munitions Compounds to Rodents

Compound	Rat mg/kg[a] (route)	Mouse mg/kg[a] (route)	Reference
TNT	800-1300 (oral)	600-1000 (oral)	214
DNT	200-800 (oral)	1200-2000 (oral)	215
NG	500-900 (oral)	500-1200 (oral)	216
	100-110 (ip)	100-200 (ip)	216
	25-32 (iv)	10-18 (iv)	216
	500-600 (sc)	30-500 (sc)	216
RDX	40-300 (oral)	60-500 (oral)	201
		19 (iv)	201
HMX	6250 (oral)	2300 (oral)	217
		634 (sc)[b]	207
NQ	>5000 (oral)	5000 (oral)	195,208,209
TNB	450 (oral)	572 (oral)	63
		32 (iv)	63
DNB	83 (oral)	200 (ip)[c]	63
DEGDN	700-1000 (oral)[d]	1300-1400 (oral)[d]	218
	777 (oral)		63
EGDN	616 (oral)		63
PGDN	250 (oral)		63
	479 (ip)	1047 (ip)	63
	463 (sc)	1208 (sc)	63
PA		100 (oral)[e]	63
Tetryl		5000 (sc)[f]	63

a. LD50 unless noted otherwise.
b. In rabbit.
c. LDLo.
d. LD100.
e. LDLo in guinea pig.
f. LDLo in dog.

Table 7. NOEL for Selected Munitions Compounds Estimated from Chronic and Subchronic Toxicity Data

Compound	Duration of Test	NOEL (mg/kg/day)	Species	Reference
TNT	13 wk	1.0[a]	rat	219
	13 wk	1.4-1.45[b]	rat	220
	13 wk	1.45-1.6[b,c]	mouse	220
	13 wk	0.2	dog	220
	26 wk	0.5[d]	dog	221
	2 yr	0.4	rat	222
DNT	1 yr	13.5	mouse	223,224
	1-2 yr	0.6	rat	223,225
	2 yr	0.2	dog	223
NG	13 wk	25.5	rat	226
	1 yr	1.0	dog	227
	2 yr	3-4[b]	rat	227
	2 yr	10-11[b]	mouse	227
RDX	13 wk	15	rat	202
	13 wk	80	mouse	202
	13 wk	1.0	monkey	202
	2 yr	0.3	rat	228
	2 yr	1.5	mouse	229
HMX	13 wk	50-115	rat	207
PA	2 yr	25[e]	rat	230
NQ	13 wk	316	rat	210
DNB	16 wk	0.75	rat	231,232
PETN	1 yr	2	rat	196

a. 5% reduction in weight gain.
b. Males and females were given slightly different doses.
c. Enlarged spleens and hearts.
d. Mild liver lesions observed in 7 of 12.
e. Calculated from concentration in feed (500 ppm), assuming standard animal weight (200 g) and feed consumption (10 g/day)[63].

Appendix F2
TNT

Source: in Chapter 3.0 - Toxicity Assessment, Section 3.1 - Nitroaromatics, U.S. Army Environmental Health Agency (USAEHA) document.

3.0 TOXICITY ASSESSMENT

3.1 NITROAROMATICS

3.1.1 TNT

2,4,6-TNT is a munitions compound currently used for commercial and military purposes. TNT is only slightly soluble in water; the reported solubility is 150 mg/L at 25°C (USABRDL, 1989). Coupled with an estimated soil sorption coefficient (K_{oc}) value of 525, which indicates soil sorption will be negligible, TNT is expected to be mobile in the soil/groundwater system with little retardation in subsurface and sandy soils. With an estimated vapor pressure of approximately 5.5 x 10^{-6} millimeters of mercury (mmHg) at 25°C, TNT is not volatile, and movement through air-filled pores in near-surface soils is presumed to be an insignificant migration pathway. The major pathway for movement into the environment is by surface water runoff and the discharge of waste streams.

Neither oxidation nor nonmicrobial hydrolysis has been identified as an important degradation pathway for TNT [U.S. Army Biomedical Research and Development Laboratory (USABRDL), 1989]. Photolysis of TNT in aquatic environments has proven to be a primary degradation pathway. Subject to seasonal and latitudinal differences, the summer half-life period is reported to be 14 hours, and the winter half-life varies from 22 days at a latitude of 2O°N to 84 days at 50°N (USABRDL, 1987). Microbial hydrolysis occurs, but at a rate significantly slower than photolysis: 19 to 25 days with a lag time of up to 20 days [Hazardous Substances Data Bank (HSDB), 1990]. TNT undergoes biotransformation but not biodegradation because, in the end product, all of the nitro groups are reduced to amino groups (USABRDL, 1987). Similar reductive

transformations by thermophilic microorganisms under composting conditions have been reported (USABRDL, 1990).

3.1.1.1 Health Effects Assessment

EPA [Integrated Risk Information System (RIS) 1990] has derived a chronic oral reference dose (RfD) of 0.0005 mg/kg/day. No interim inhalation or subchronic oral RfDs are available (HEAST, 1990). The chronic oral RfD was derived from a 26-week study in which dogs were dosed via gelatin capsule at 0, 0.5, 2, 8, or 32 milligrams per kilogram per day (mg/kg/day) (IRIS, 1990). Increased liver weight in conjunction with hepatic swelling and hepatocytomegaly was observed in male dogs receiving 8 or 32 mg/kg/day; these effects were only observed in the female rats receiving the 32 mg/kg/day. Although hepatic swelling and hepatocytomegaly were observed at all dose levels, they were described as trace to mild in the lowest dose group (IRIS, 1990). Hemosiderosis of the liver was observed in **a** majority of animals receiving doses of 2 and 8 mg/kg/day, and microscopic evidence of cirrhosis was observed at the 8 and 32 mg/kg/day level (IRIS, 1990). Based on this study, a value of 0.5 mg/kg/day was identified as the lowest-observed-adverse-effect level (LOAEL) based on potential liver toxicity.

EPA has classified TNT as a group C (possible human) carcinogen (IRIS, 1990), which indicates that insufficient data are available regarding TNT's carcinogenicity in humans. Limited evidence of TNT's carcinogenic effects in experimental animals is available. In a 2-year rat feeding study, hepatocellular (male rats) and renal and urinary bladder hyperplasia (female rats) were observed in addition to bladder carcinoma and transitional cell papilloma in animals exposed to a daily dose of 10 mg/kg/day or greater (IRIS, 1990). No

significant change in neoplasms were reported in mice dosed at levels as high as 70 mg/kg/day (IRIS, 1990).

Human toxicity data consist primarily of data from munitions worker studies. Pathological manifestations have been reported as dermatitis, gastritis, and acute yellow atrophy of the liver, as well as petechial hemorrhages; aplastic anemia in older workers and toxic hepatitis in younger workers; nephritis; severe irritation and erythema of the skin; and headache, fatigue, and drowsiness associated with cyanosis. In severe cases, anuria, delirium, convulsions, and coma may occur (HSDB, 1990). Ocular damage may also be manifested, as evidenced by cataracts in a large number of occupationally exposed workers (HSDB, 1990).

In an acute study, dogs were dosed at 0, 0.2, 2.0, or 20 mg/kg/day for 13 weeks; rats received diets containing 0.002-, 0.01-, 0.05- or 0.25-percent TNT; and mice received diets with 0.00l-, 0.005-, 0.025-, or 0.125-percent TNT over the same period (HSDB, 1990). The highest dose caused anemia in all species and increased organ weights (the latter were temporary in dogs and mice). Alterations were seen in most clinical chemistry parameters, and reduced testes size was seen in rats at the highest dose regardless of length of exposure. All effects were reversible except for the testicular atrophy. When injected intraperitoneally into male rats at 100 mg/kg, TNT caused damage in the cerebral, hepatic, and renal biomembranes, and in cell organelles.

In a chronic feeding study in which rats were subjected to a 24-month dosing regimen of 0.4, 2, 10, or 50 mg/kg/day, a no-observed-adverse-effect level (NOAEL) of 0.4 mg/kg/day was established based on an absence of effects to

the spleen, kidney, bone marrow, and the bladder at that dose (IRIS, 1990). In a subchronic feeding study using dogs, rats, and mice, dogs were the most sensitive with effects reported at 2 mg/kg/day, although no effects were reported at 0.2 mg/kg/day. In the rats, toxic effects were reported at 7 mg/kg/day (male) and 7.4 mg/kg/day (female);. in mice, no toxicity was reported until reaching a dose of 35.7 mg/kg/day (male) and 37.8 mg/kg/day (female) (IRIS, 1990).

TNT was mutagenic to three Salmonella typhimurium strains, with or without metabolic activation. However, rats treated for 28 days, with TNT up to 1.8 mgfkg/day evidenced no in vivo genetic damage (IRIS, 1990). No teratogenic or other reproductive effects have been reported, but testicular atrophy was reported in male rats following doses of 25, 125, and 300 mg/kg/day for 13 weeks. The importance of the latter effect is questioned as it was not duplicated in any other species and is a common response of rats to any toxic insult [IRIS, 1990; Oak Ridge National Laboratory (ORNL), 1987]. A NOAEL of S mg/kg/day is indicated by the absence of testicular degeneration and effects on the spleen at this dose level (IRIS, 1990).

3.1.1.2 Ecotoxicity

Aquatic Organisms

Several algal species, but no vascular plant species, were tested to evaluate short-term effects; Table 3.1-1 presents a summary of the results. Following 24 hours of exposure to 8 mg/L of TNT, loo-percent mortality **was** reported in the algae Microcystis aeruginosa (Fitzgerald et. al., 1952). Following exposure of Selenastrum capricomutum to TNT for 7 days, 2.5 mg/L was found to significantly reduce growth, and 10 mg/L was lethal (Won et. al., 1976).

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Table 3.1-1. Acute Toxicity of 2,4,6-TNT to Aquatic Organisms

Scientific Name (Common Name)	Effect	S/F	Duration (hours)	Concentration (mg/L)	Reference
INVERTEBRATES					
Lumbriculus variegatus (oligochaete)	LC50	S	48	5.2	Liu et al., 1983a (LLNL, 1987)
	LC50	F	96	>29.0 (M)	Liu et al., 1983a (LLNL, 1987)
Daphnia magna waterflea)	LC50	S	48	11.7 (M)	Liu et al., 1983a (LLNL, 1987)
	LC50	F	96	1.2 (M)	Liu et al., 1983a (USABRDL, 1989)
	LC50	S	48	11.9	Liu et al., 1983b (LLNL, 1987)
	LC50	F	48	6.6	Liu et al., 1976 (LLNL, 1987)
	LC50	S	48	0.8*	Liu et al., 1983c (LLNL, 1987)
Hyalella azetca (Scud)	LC50	S	48	6.5	Liu et al., 1976 (LLNL, 1987)
	LC50	F	96	6.5	Liu et al., 1976 (LLNL, 1987)
Tanytarsus dissimilis (Midge)	LC50	S	48	27.0	Liu et al., 1983a (LLNL, 1987)
VERTEBRATES					
Oncorhyncus mykiss (was Salmo gairdneri)	LC50	S	96	0.8	Liu et al., 1983a (USABRDL, 1989)
(Rainbow trout)	LC50	S*	96	1.4	Liu et al., 1983a (USABRDL, 1989)
	LC50	F	96	2.0 (M)	Liu et al., 1983a (USABRDL, 1989)
Pimephales promelas (Fathead minnow)	LC50	S	96	2.9	Liu et al., 1983a (USABRDL, 1989)
	LC50	F	96	3.7(M)	Liu et al., 1983a (USABRDL, 1989)
	LC50	S	96	2.0	Liu et al., 1976 (USABRDL, 1989)
	LC50	F	96	2.9	Liu et al., 1983a (LLNL, 1987)
	LC50	F	96	2.58	Smock et al., 1976 (LLNL, 1987)
	LC50	S	96	2.9	Liu et al., 1983a (LLNL, 1987)
	EC50	F	96	0.46	Smock et al., 1976 (LLNL, 1987)

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Table 3.1-1. Acute Toxicity of 2,4,6-TNT to Aquatic Organisms (Continued, Page 2 of 2)

Scientific Name (Common Name)	Effect	S/F	Duration (hours)	Concentration (mg/L)	Reference
VERTEBRATES (Cont'd.)					
Pimephales promelas (Fathead minnow)	LC5O	S	96	3.0	Liu et al., 1983b (LLNL, 1987)
	LC5O	S	96	0.1*	Liu et al., 1983c (LLNL, 1987)
Lepomis macrochirus (Bluegill)	LC5O	S	96	2.6	Liu et al., 1983a (USABRDL, 1989)
	LC5O	S+	96	3.4	Liu et al., 1983a (USABRDL, 1989)
	LC5O	F	96	2.5 (M)	Liu et al., 1983a (USABRDL, 1989)
Ictarus punctatus (Channel catfish)	LC5O	S	96	2.4	Liu et al., 1983a (USABRDL, 1989)
	LC5O	F	96	3.3 (M)	Liu et al., 1983a (USABRDL, 1989)
	LC5O	F+	96	2.4	Liu et al., 1983a (USABRDL, 1989)

Note: EC50 = median effective concentration (Moribund response based on three behavioral responses: shock, loss of motor control, and loss of equilibrium).
LC5O = lethal concentration (lethal for SO percent of exposed group).
M = measured concentration; all others are assumed to be nominal concentrations.
S/F = static or flow-through test.

References in parentheses are secondary sources.

*Test was completed using 2,3,6-TNT.
+Static test containers were aerated during testing.

Source: ESE.

Bringmann and Kuehn (1980) found that cell multiplication was inhibited when Scenedesmus quadricauda, incubated at 27°C was exposed to TNT for 24 hours. Based on the decreased growth, the toxicity threshold was determined to be 1.6 mg/L.

Several aquatic invertebrate species have been tested to determine the acute toxicity of TNT. The results of individual tests, which were performed either as static or flow-through, are presented in Table 3.1-1 with corresponding references. The static 48-hour LC5O values reported for Daphnia manna, representing freshwater invertebrates, are 11.7 and 11.9 mg/L, and a measured 48-hour value of 6.6 mg/L was reported for one flow-through test. A measured value of 1.2 mg/L was reported for a 96-hour flow-through test. In addition to testing the 2,4,6-isomer, the 2,3,6-isomer was tested in a static 48-hour test with a resultant LC5O value of 0.8 mg/L reported. Other species tested include the asellid Hyalella azetca (scud), the chironomid Tanytarsus dissimilis (midge), and the oligochaete Lumbriculus variegatus (worm). Static 48-hour LC5O values reported for these species were 6.5 mg/L, 27.0 mg/L, and 5.2 mg/L, respectively; a measured 48-hour flow-through LC5O value of 29.0 mg/L was reported for L. variegatus.

The acute toxicity of 2,4,6-TNT to several species of vertebrate organisms has been studied (see Table 3.1-1). An evaluation of the effect of water hardness and temperature on the toxicity of TNT to Lepomis macrochirus (bluegill sunfish) found that water hardness was not a factor but that toxicity was lower at 10°C than at 25°C (see Table 3.1-1) (Pedersen, 1971). A study by Liu et. al., (1976) using Pimephales promelas (fathead minnow) found that the 96-hour LC5O increases as the pH increases, and toxicity decreases as TNT is

photodegraded [Lawrence Livermore National Laboratory (LLNL) 1987]. LC5O values for two species in addition to the bluegill and the fathead minnow have been determined. The species are Oncorhyncus mykiss (former taxonomic designation was Salmo gairdneri) or rainbow trout, and Ictarus punctatus or channel catfish. Table 3.1-2 includes a summary of the acute tests and the corresponding references. In response to static 96-hour tests, the rainbow trout, with reported LC5O values ranging from 0.8 mg/L to 1.4 mg/L, appears to be the most sensitive of the four species tested. Static 96-hour LC5O values for TNT ranged from 2.0 to 2.9 mg/L for the fathead minnow, 2.6 to 3.4 mg/L for the bluegill, and a single value of 2.4 mg/L is listed for the channel catfish. in addition to the static tests, results of 96-hour flow-through tests, many of which are measured values, are available for the same four species. As with the static test results, the rainbow trout is the most sensitive, with a measured value of 2.0 mg/L reported. For the fathead minnow, a measured value of 3.7 mg/L is reported, and nominal concentrations of 2.58 and 2.9 are reported. A measured value of 2.5 mg/L is reported for the bluegill, and the nominal and measured values reported for the channel catfish are 2.4 and 3.3 mg/L, respectively. As part of their studies, Liu et. al., (1983a) determined an LC5O value of 0.1 mg/L in the fathead minnow for 2,3,6-trinitrotoluene (2,3,6-TNT), indicating that this isomer is approximately 10 times more toxic than the 2,4,6-isomer.

Several algal species were studied in terms of longer exposure to TNT. Following a 17-day exposure, growth inhibition was reported in Selenastrum capricomutum at a concentration of 5 mg/L (Smock et al., 1976), and a value of 4.1 mg/L was reported by Liu et al., (1983a) to inhibit growth after a 14-day exposure period. Growth inhibition was reported by Liu et al., (1983a)

Table 3.1-2. Chronic Toxicity of 2,4,6-TNT to Aquatic Organisms

Scientific Name (Common Name)	Effect	S/F	Duration (hours or days)	Concentration (mg/L)	Reference
ALGAE					
Selenastrum capricomutum	Growth inhibition	--	14 days	4.1	Liu et al., 1983a (ORNL, 1987)
	Growth inhibition	--	17 days	5	Smock et al., 1976 (LLNL, 1987)
	Growth inhibition	--	7 days	2.5	Won et al., 1976 (ORNL, 1987)
	Death	--	2 days	10	Won et al., 1976 (ORNL, 1987)
Microcystis aeruginosa	Growth inhibition	--	17 days	15	Smock et al., 1976 (LLNL, 1987)
	Growth inhibition	--	14 days	4.1	Liu et al., 1983a (ORNL, 1987)
	Death (100%)	--	24 hr	8	Fitzgerald et al., 1952 (ORNL, 1987)
Anabaena flos-aqua	Growth inhibition	--	14 days	8.2	Liu et al., 1983a (ORNL, 1987)
Naviculla pelliculosa	Growth inhibition	--	14 days	18	Liu et al., 1983a (ORNL, 1987)
Scenedesmus quadricauda	Toxicity threshold	--	16 hr	1.6	Bringmann and Kuehn, 1980 (ORNL, 1987)
PLANTS					
Lemna perpusilla (Duckweed)	Growth inhibition	--	11 days	1.0*	Schott and Worthley, 1974 (USABRDL, 1989)
	Death	--	11 days	5.0*	Schott and Worthley, 1974 (USABRDL, 1989)
	NEC	--	11 days	≤0.5 (M)	Schott and Worthley, 1974 (USABRDL, 1989)

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Table 3.1-2. Chronic Toxicity of 2,4,6-TNT to Aquatic Organisms (Continued, Page 2 of 2)

Scientific Name (Common Name)	Effect	S/F	Duration (hours or days)	Concentration (mg/L)	Reference
INVERTEBRATES					
Daphnia magna (Waterflea)	Incipient LC50	F	192 hr	0.2 (M)	Liu et al., 1983a (USABRDL, 1989)
	Incipient LC50	F	336 hr	0.19 (M)	Liu et al., 1983a (USABRDL, 1989)
	Reproductive	F		1.03	Bailey et al., 1985 (USABRDL, 1989)
VERTEBRATES					
Oncorhyncus mykiss (Rainbow trout)	Incipient LC50	F	240 hr	1.9 (M)	Liu et al., 1983a (USABRDL, 1989)
	ELS, fiy survival	--		0.24	Bailey et al., 1985 (USABRDL, 1989)
Pimephales promelas (Fathead minnow)	Incipient LC50	F	14 day	1.4 to 1.9	Liu et al., 1983a (USABRDL, 1989)
	Incipient LC50	F	192 hr	1.5 **(M)**	Liu et al., 1983a (USABRDL, 1989)
	ELS, repro-ductive	F	90 day	0.04	Bailey et al., 1985 (USABRDL, 1989)
Lepomis macrochirus (Bluegill)	Incipient LC50	F	14 day	1.4 to 1.9	Liu et al., 1983a (LLNL, 1987)
	Incipient LC50	F	312 hr	1.4 (M)	Liu et al., 1983a (USABRDL, 1989)
lctarus punctatus (Channel catfish)	LC50	F	288 hr	1.6 (M)	Liu et al., 1983a (USABRDL, 1989)

Note: ELS = early life stage.
M = measured.
NEC = no-effect concentration.
ORNL = Oak Ridge National Laboratory.
S/F = static or flow-through test conditions.
.. = test conditions not specified.

References in parentheses are secondary sources.

*Test completed with 2,3,6-TNT.

Source: ESE.

in M. aeruginoisa at a concentration of 4.1 mg/L following a 14-day exposure. Smock et al., (1976) reported growth inhibition at 15 mg/L following a 17-day exposure. Growth inhibition was also reported in Anabaena flos-aquae following 14 days of exposure to 8.2 mg/L and in Navicula pelliculosa after a 14-day exposure to 18 mg/L (Liu et al., 1983a). Following an 11-day exposure of duckweed, or Lemna perpusilla, to TNT in a hydroponic solution, growth inhibition was reported at a concentration of 1.0 mg/L, and death was reported at 5.0 mg/L (Schott and Worthley, 1974).

In the testing of invertebrates, a parameter known as the incipient LC5O is reported; this term signifies the concentration at which 50 percent of the exposed population would expire following an indefinite exposure. The measured incipient flow-through values reported for D. magna are 0.2 mg/L following a 192-hour exposure and 0.19 mg/L following a 336-hour exposure (Liu et al., 1983a). A value of 1.03 mg/L was reported by Bailey et al. (1985) as the flow-through concentration at which reproductive effects were observed in D. magna. Chronic toxicity test data are presented in Table 3.1-2.

The bioconcentration potential of TNT in several aquatic species was evaluated by Liu et al., (1983a). Following a 96-hour exposure, a bioconcentration factor (BCF) of 453 was reported for the algae, S. capricomutum, and a whole body BCF of 209 was reported for D. magma. In vertebrates, Liu et al., (1983a) reported a 96-hour BCF of 338 in the viscera of the bluegill, but the muscle BCF was measured at 9.5. Because these values were determined from data collected during the uptake process prior to reaching a steady state, the authors estimated a steady state whole body BCF value of 20.5. In its evaluation of munitions, USABRDL (1989) estimated a BCF value of 8.95 for fish, and

Layton et al., (1987) estimated a BCF value of 7 for fish. In 1983, Xu and Chen investigated the bioconcentration of TNT in a microcosm consisting of Tilapia mossambica (fish), Belbamya purificata, Pista stratiotes (water lettuce), and Anlirrhinum majus. The resulting calculated dry weight BCF values were reported as 210; 171; 1,165 to 1,415; and 1,623 to 2,030, respectively (LLNL, 1987). BCF data are presented in Table 3.1-3.

Terrestrial Organism

Few toxicity tests with terrestrial plants have been reported. One study by Palazzo and Leggett (1986) reported on the effects of TNT on yellow nutsedge grown in a hydroponic solution. At a concentration of 5 mg/L TNT, root weight was reduced by 95 percent. Visible symptoms of root injury included discoloration and growth restriction.

No studies concerning TNT toxicity to wildlife were found in the literature; however, toxicological studies using laboratory animals may serve as models for wildlife species. These studies indicate that, in small doses, TNT is rapidly detoxified and excreted. In acute studies reported by ORNL (1987), lethal dose (lethal for 50 percent of exposed group) (LD5O) values ranged from 794 to 3,190 milligrams per kilogram (mg/kg) for rats and 660 to 1,014 mg/kg for mice; in one study on rabbits, the LD5O value was 940 mg/kg (Table 3.1-4).

In chronic studies, dogs and monkeys exposed to less than 1 mg/kg/day for 90 days showed no toxic effects (ORAL, 1987); however, dogs dosed with 7 mg/kg of TNT twice a week for 9 months showed renal pathological changes. In additional studies reported by ORNL (1987), gastric disorders were reported in dogs exposed to TNT dosages as low as 0.1 mg/kg for 1.5 to 2.5 years.

Table 3.1-3. Bioconcentration Factors* for TNT

Species Name	Tissue	BCF	Reference
Fish (general)		7 (E) 8.95 (E)	LLNL, 1987 (USABRDL, 1989)
Lepomis macrochims (Bluegill)	viscera	338	Liu et al., 1983a (ORNL, 1987)
96 hr uptake	muscle	9.5	Liu et al., 1983a (ORNL, 1987)
(Steady State)	whole body	20.5 (E)	Liu et al., 1983a (ORNL, 1987)
Tilapia mossambica	NS	210	Xu and Chen, 1983 (ORNL, 1987)
Selenastrum capricomutum (96 hr)	NS	453	Liu et al., 1983a (ORNL, 1987)
Belbamya purificata	NS	171	Xu and Chen, 1983 (ORNL, 1987)
Pistia stratiotes (Water lettuce)	NS	1,165 to 1,415	Xu and Chen, 1983 (ORNL, 1987)
Anlirrhinum major	NS	1,623 to 2,030	Xu and Chen, 1983 (ORNL, 1987)
Lumbriculus variegatus (Oligochaete) (96 hr)	whole body	202	Xu and Chen, 1983 (OWL, 1987)

Note: E = estimated.
NS = not specified.

References in parentheses are secondary sources.

*Unitless.

Source: ESE.

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Table 3.1-4. Acute Toxicity* of 2, 4, 6-TNT

Test Species	LD5O Value mg/kg)	Reference
Rat	1,014	Lee et al., 1975
Rat	820	Lee et al., 1975
Rat	3,190	Vasilenko and Kovalenko, 1976
Rat	1,320	Dilley et al, 1978
Rat	794	Dilley et al., 1978
Mouse	1,014	Lee et al., 1975
Mouse	1,009	Lee et al., 1975
Mouse	680	Vasilenko and Kovalenko, 1976
Mouse	830	Newell et al., 1976
Mouse	660	Dilley et al., 1978
Rabbit	940	Vasilenko and Kovalenko, 1976

*Oral dose by gastric intubation with test material suspended in corn or peanut oil; animals were fasted for 16 hours before testing and and observed for 14 days past treatment.

Source: ORNL, 1987.

In studies using rats and mice, rats administered TNT for up to 24 months displayed anemia, hepatotoxicity, and urogenital lesions (ORNL, 1987). Hyperplastic and/or neoplastic lesions of the liver, kidneys, and urinary bladder also were observed at doses of 10 mg/kg/day or greater. The observed carcinoma of the urinary bladder indicates that TNT is a carcinogen to rats under the experimental conditions.

Table 3.1-5 summarizes the results of several chronic studies with 2,4,6-TNT and laboratory mammals. No-observed-effect level (NOEL) values range from 0.4 to 1.45 mg/kg in rats and 0.5 mg/kg in dogs. LOAEL values are reported as 1.45 to 1.6 mg/kg in mice, and lowest-observed-effect level (LOEL) values are reported as 0.5 mg/kg for dogs and rabbits. Only two BCF values were found in the literature. USABRDL (1989) reported an estimated value of 0.0013 for beef (general), and LLNL (1987) reported an estimated value of 0.0026 for beef (general).

3.1.1.3 Criteria and Standards

Current data for calculating water quality criteria are insufficient to meet all EPA guidelines. However, using calculations from previous EPA guidelines, a reasonable estimate of the criterion maximum concentration to protect aquatic life is 557 μg/L; the criterion for continuous concentration is tentatively estimated at 40 μg/L (ORNL, 1987). No ambient water quality criteria (AWQC) currently exist for TNT.

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Table 3.1-5. Chronic Toxicity of 2,4,6-TNT

Species	Effect	Duration	Dose (mg/kg/day)	Reference
Rat	NOEL	13 weeks	1.0	Levine et al., 1984 (USABRDL, 1989)
	NOEL	13 week	1.4 to 1.45	Dilley et al., 1978 (USABRDL, 1989)
	NOEL	2 years	0.4	Furedi et al., 1984 (USABRDL, 1989)
Mouse	LOAEL	13 weeks	1.45 to 1.6	Dilley et al., 1978 (USABRDL, 1989)
Dog	NOEL	13 weeks	0.2	Dilley et al., 1978 (USABRDL, 1989)
	LOEL	26 weeks	0.5	Levine et al., 1983 (USABRDL, 1989)
Rabbit	LOEL	8 months	0.005	Galuzova, 1963 (USABRDL, 1974)

Source: ESE.

Appendix F3
DNT

Source: in Chapter 3.0 - Toxicity Assessment, Section 3.1 - Nitroaromatics, U.S. Army Environmental Health Agency (USAEHA) document.

3.1.2 DNT

DNT exists as any one of six isomen. In the munitions industry, only two isomers are commonly found: 2,4-dinitrotoluene (2,4-DNT) and 2,6-dinitrotoluene (2,6-DNT). These compounds are ingredients of explosives used by commercial and military personnel and are also used as stabilizers in the manufacture of smokeless powder (EPA, 1980).

The estimated soil adsorption coefficient (K_{oc}) values for 2,4-DNT and 2,6-DNT are 251 and 78, respectively (USABRDL, 1989), indicating that there will negligible sorption to soil. Coupled with estimated water solubilities of 280 and 206 mg/L at 25°C (USABRDL, 1989), 2,4-DNT and 2,6-DNT are expected to be mobile in the soil/groundwater system with little retardation in subsurface and sandy soils. With estimated vapor pressures of 0.000217 and 0.000567 mmHg at 25°C for 2,4-DNT and 2,6-DNT, respectively (USABRDL, 1989), these compounds are not volatile. Consequently, movement through the air-filled pores in near-surface soils is presumed to be an insignificant migration pathway.

No evidence exists for other chemical transformation processes, such as hydrolysis or oxidation, under environmental conditions (USABRDL, 1989). The DNTs may be biodegraded or at least biotransformed, as the nitro groups are reduced under aerobic conditions to ammo- and azoxyaromatic compounds (USABRDL, 1989).

3.1.2.1 Health Effects Assessment

No oral or inhalation RfDs have been developed for either 2,4-DNT or 2,6-DNT; EPA indicates that the available data are insufficient for quantitative risk assessment [Health Effects Assessment Summary Tables (HEAST) 1990].

EPA has classified both 2,4-DNT and 2,6-DNT as group B2 (probable human) carcinogens (HEAST, 1990). Bats were exposed to a dietary mixture of the two isomers for a 2-year period, following which liver and mammary tumors were reported (HEAST, 1990). Based on the data generated from this study, an oral cancer slope factor of 0.68 $(mg/kg/day)^{-1}$ was calculated (HEAST, 1990). No inhalation cancer slope factor was developed. The results of a feeding study using rats that were dosed with diethylnitrosamine as a hepatic initiator-promotor indicated that 2,4-DNT and 2,6-DNT are hepatocarcinogens but that the 2,6-DNT isomer is 10 times more potent than the 2,4-DNT isomer (HSDB, 1990).

The primary result of acute exposure is the formation of methemoglobin leading to cyanosis (EPA, 1980). In order of probable occurrence, the following symptoms are reported in humans exposed to the DNTs (HSDB, 1990). First, signs of cyanosis as evidenced by a darkening of the tongue, lips, mucous membranes, and skin with no signs of cardiac or pulmonary insufficiency. This is followed by headache and nausea that can include vomition, then by CNS effects including ataxia, weakness, disorientation, confusion, lethargy, and finally coma; convulsions may occur but are not common. In a similar timeframe postexposure, cardiac effects may be observed that include heart blocks, arrhythmias, and shock. When death does occur, which is not common, it is usually due to cardiovascular collapse (HSDB, 1990). A study of workers

exposed to DNT or toluene diamine found no significant increase in cancer but did find an increase in mortality due to ischemic heart disease.

Male rats orally administered technical grade DNT for a S-day period evidenced markedly elevated microsomal cytochrome P-450-dependent enzyme activities; no other effects were reported (HSDB, 1990). Rats exposed to 34 (males) or 38 mg/kg/day (females) for 13 weeks evidenced depressed weight gain, Doses of 93 and 108 mg/kg/day, respectively, were toxic, with evidence of splenic hemosiderosis and decreased spermatogenesis (HSDB, 1990). In a 2-year rat feeding study, levels of 0.57 (males) and 0.71 mg/kg/day (females) evinced no apparent toxic effect. The next higher dose of 3.9 (males) and 5.1 mg/kg/day (females) was toxic, evidencing depressed spermatogenesis (males) and numerous carcinomas (both sexes) (HSDB, 1990). The mouse is observed to be much more tolerant following exposure to any of the DNT compounds alone or in combination (HSDB, 1990). The compounds 2,4-DNT; 2,6-DNT, and 34-DNT are substantially more toxic than the other isomers (HSDB, 1990).

Technical-grade 2,4-DNT (76.5 percent 2,4-DNT and 18.8 percent 2,6-DNT) was mutagenic with several Salmonella typhimurium strains, particularly in strains that respond to frame-shift mutagens (HSDB, 1990). A separate mutagenic study using S strains of Salmonella typhimurium found that the enzyme nitroreductase was necessary to induce mutation (HSDB, 1990). Both 2,4-DNT and 2,6-DNT were identified as genotoxic, with the potency of the 2,6-isomer much greater than that of the 2,4-isomer (HSDB, 1990).

3.1.2.2 Ecotoxicity

Aquatic Organisms

Several studies have been completed to assess the toxicity of several isomers of DNT to freshwater algae, plants, and invertebrate and vertebrate organisms. The results are presented in Table 3.1-6, and many results are also available in the Ambient Water Quality Criteria for Dinitrotoluene document prepared by EPA (1980d). No AWQC are available for the DNT isomers; however, EPA (1980d) states that acute and chronic toxicity occur at concentrations as low as 330 µg/L and 230 µg/L, respectively, and would occur at lower concentrations in species that are more sensitive than those tested.

Most of the isomers have been evaluated in terms of their potential toxicity to freshwater aquatic organisms (Liu et al., 1983a). The studies consist of 48-hour static LD50 studies using Daphnia magna and 96-hour static LD50 studies using Pimephales promelas (fathead minnow). Other studies were completed using the algae Selenastrum capricornutum and Lepomis macrochirus (bluegill). The results presented in Table 3.1-6 indicate that the 2,3-DNT, 2,5-DNT, and 3,4-DNT isomers are about 10 times more toxic than the 2,4-DNT, 2,6-DNT, or 3,5-DNT isomers. EPA (1980d) reports a SO-percent reduction in cell numbers and chlorophyll a after a 96-hour exposure at levels of the 2,3-DNT isomer that are approximately equal to the 2,3-DNT LD5O values reported in the fathead minnow (Liu et at., 1983a). BCF data are presented in Table 3.1-7.

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Table 3.1-6. Toxicity of DNT Isomers to Aquatic Organisms

Scientific Name (Common Name)	Isomer	Effect	S/F	Duration (hours or days)	Concentration (mg/L)	Reference
ALGAE						
Selenastrum capricornutum	2,3-	SO%	Growth Inhibition		1.37	EPA 1980d
(Blue-green algae)	2,3-	SO%	Inhibition of chlorophyll a		1.62	EPA, 1980d
PLANTS						
Lemna perpusilla (Duckweed)	2,4-	NEC	S	11 days	0.1 to 0.5	Schott and Worchley, 1974 (USABRDL, 1989)
INVERTEBRATES						
Daphnia magna	2,4-	LC5O	S	48 hr	47.5	Liu et al., 1983a (LLNL, 1987)
	2,6-	LC5O	S	48 hr	21.8	Liu et al., 1983a (LLNL, 1987)
	3,5-	LC5O	S	48 hr	45.2	Liu et al., 1983a (LLNL, 1987)
	3,4-	LC5O	S	48 hr	3.7	Liu et al., 1983a (LLNL, 1987)
	2,3-	LC5O	S	48 hr	4.7	Liu et al., 1983a (LLNL, 1987)
	2,5-	LC5O	S	48 hr	3.1	Liu et al., 1983a (LLNL, 1987)
	2,4-	EC5O	S	48 hr	35	EPA, 1980d
	2,6-	EC5O	S	48 hr	21.8	Liu, et al., 1983b (LLNL, 1987)
	2,3-	EC5O	S	48 hr	0.66	EPA, 1980d
VERTEBRATES						
Pimephales promelas (Fathead minnow)	2,4-	LC5O	S	96 hr	32.8	Liu, et al., 1983a (LLNL, 1987)
	2,6-	LC5O	S	96 hr	18.5	Liu, et al., 1983a (LLNL, 1987)
	3,5-	LC5O	S	96 hr	22.6	Liu, et al., 1983a (LLNL, 1987)
	3,4-	LC5O	S	96 hr	1.5	Liu, et al., 1983a (LLNL, 1987)
	2,3-	LC5O	S	96 hr	1.8	Liu, et al., 1983a (LLNL, 1987)
	2,5-	LC5O	s	96 hr	1.3	Liu, et al., 1983a (LLNL, 1987)

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Table 3.1-6. Toxicity of DNT Isomers to Aquatic Organisms (Continued, Page 2 of 2)

Scientific Name (Common Name)	Isomer	Effect	S/F	Duration (hours or days)	Concentration (mg/L)	Reference
VERTEBRATES (Cont'd.)						
Pimephales promelas (Fathead minnow)	2,4-	LC50	--	96 hr	31	EPA, 1980d
	ND	LC50	--	chronic	0.28	USABRDL, 1989
	2,3-	Embryo-larval	--	--	0.23	EPA 1980d
Lepomis macrochirus (Bluegill)	2,3-	LC50	S	96 hr	0.33	EPA, 1980d

Note: ND = isomer not provided.
-- = no pertinent information provided.

References in parentheses are secondary sources.

Source: ESE.

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Table 3.1-7. Bioconcentration Factors* for DNT

Species Name	Tissue	BCF	Reference
2,4-DNT			
Fish (general)	muscle	10.6	Hartley, 1981 (LLNL, 1987)
		11.6 (E)	USABRDL, 1989
		3.8 (E)	EPA, 1980d
		15 (E)	LLNL, 1987
		78	Liu et al., 1983a (LLNL, 1987)
	brain	103	Hartley, 1981 (LLNL, 1987)
	whole body	24.8	Hartley, 1981 (LLNL, 1987)
Beef (far/feed)		0.0034 (E)	USABRDL, 1989
		0.0027 (E)	LLNL, 1987
Daphnia magra		13	Liu et al., 1983c (LLNL, 1987)
Algae (unspecified)		5,225	HSDB, 1990
Selenastrum capricornutum		2,507	Liu et al., 1983a (LLNL, 1987)
2,6-DNT			
Fish (general)	muscle	9.82 (E)	USABRDL, 1989
		13 (E)	LLNL, 1987
Carp	muscle	19 (E)	HSDB, 1990
Beef (fat/feed)		0.0031 (E)	USABRDL, 1989; LLNL, 1987

Note: E = estimated.

References in parentheses are secondary sources.

*Unitless.

Source: ESE.

Terrestrial Organisms

Data for the toxicity of DNT to terrestrial wildlife must be inferred from tests conducted with laboratory mammals because tests have not been conducted with wildlife species. In subacute toxicity studies of 2,4-DNT, dogs were fed daily doses of 1, 5, or 25 mg/kg, and rats and mice were fed doses of 0.07, 0.2, or 0.7 percent of feed for 13 weeks. The highest doses were lethal to some animals in all three species, and the lowest doses produced no toxic effects (EPA, 1980d). All species exhibited methemoglobinemia and anemia. The toxicity of DNT isomers to laboratory animals is presented in Table 3.1-8.

The effects of chronic exposure to 2,4-DNT include liver damage, jaundice, and reversible anemia (EPA, 1980d). Bats fed a technical-grade mixture of DNT (2,4-DNT and 2,6-DNT) or 2,6-DNT for 1 year developed liver cancer (HSDB, 1990). BCF data are presented in Table 3.1-7.

3.1.2.3 Criteria and Standards

Insufficient data are available to develop AWQC for 2,4-DNT.

3.1.3 NITROBENZENE

The predominant use for nitrobenzene (NB) is reduction to aniline, which is then used in dyes, rubber, and medicines. NB also is used as a solvent; combustible propellant; almond essence substitute; in perfume; and in metal, floor, and shoe polishes.

NB is moderately adsorbed to soil; upon leaching into the ground or entering water systems, NB is expected to biodegrade within a few months (HSDB, 1990). In the atmosphere, the predominant degradation route is

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Table 3.1-8. Toxicity of DNT Isomers to Terrestrial Laboratory Mammals

Species	Isomer	Effect	Duration	Dose (mg/kg/day)	Reference
Rat	2,4- and 2,6-	LD5O	Oral Acute	200 to 800	Etnier, 1987 (USABRDL, 1989)
	2,4-	LD5O	Oral	268	EPA, 1980d
Mouse	2,4- and 2,6-	LD5O	Oral Acute	1,200 to 2,000	Etnier, 1987 (USABRDL, 1989)
	2,4-	NOEL	Oral	1,625	EPA, 1980
Rat	2,4-	NOEL	1 to 2 years	0.6	Ellis et al., 1979; Lee et al., 1985 (LLNL, 1987)
Mouse	2,4-	NOEL	1 year	13.5	Ellis et al., 1979; Hong et al., 1985 (LLNL, 1987)
Dog	2,4-	NOEL	2 year	0.2	Ellis et al., 1979 (LLNL, 1987)
		NOEL	2 year	10	Ellis et al., 1985 (LLNL, 1987)

Note: References in parentheses are secondary sources.

Source: ESE.

photolysis, and photoreduction has also been reported (EPA, 1979). Hydrolysis is not reported to occur for NB (EPA, 1979; LLNL, 1987). EPA (1979) reports that oxidation probably does not act as an initial aquatic fate process for NB. Volatilization is not expected to be an important migration pathway for NB because of the low vapor pressures, which are reported as 0.15 mmHg at 20°C (LLNL, 1987; EPA, 1979).

3.1.3.1 Health Effects Assessment

EPA has derived an oral chronic and interim oral subchronic RfD for NB of 0.0005 mg/kg/day (IRIS, 1990) and 0.005 mg/kg/day (HEAST, 1990), respectively. Although still listed in the IRIS database, EPA (HEAST, 1990) states that the chronic value for NB is currently being reconsidered.

in terms of exposure through inhalation, EPA (HEAST, 1990) has derived interim chronic (0.002 mg/kg/day) and subchronic (0.02 mg/kg/day) inhalation RfDs for NB. The interim chronic inhalation RfD has been verified and is pending input to the IRIS database as a final value (HEAST, 1990). These values were derived from an inhalation study in which rats and mice were exposed for 90 days to airborne NB (IRIS, 1990). Rats of both sexes evidenced an increase in hemolytic anemia, and female mice had increased vacuolization of the adrenal cells at 25 micrograms per cubic meter (mg/m^3). Liver and kidney damage was reported at the highest exposure of 81 mg/m^3. The NB oral RfD was then derived as a route-to-route extrapolation from the inhalation study (HEAST, 1990).

Data regarding effects of NB to humans are limited to occupational exposure in Which headaches, vertigo, and methemoglobinemia were the primary symptoms

reported (IRIS, 1990). Although methemoglobin is not formed as quickly by NB as by aniline, the resultant cyanosis is generally more persistent (HSDB, 1990). Other symptoms associated with the inhalation of NB are nausea, vomition, and depressed respiration that may lead to stupor; coma; and, in the most severe cases, death from respiratory failure (HSDB, 1990). Repeated exposure may lead to yellow atrophy, hemolytic icterus, and anemia of varying degrees with the presence of heinz bodies in the red blood cells; all of these symptoms are evidence of liver impairment (HSDB, 1990). Ocular effects are also reported, consisting primarily of browning of the fundus and the conjunctiva (HSDB, 1990).

CNS depression, methemoglobinemia, and marked cyanosis were also reported in experimental animals exposed to NB (HSDB, 1990). The bone marrow in rabbits evidenced changes ranging from hyperplasia to hypoplasia and even aplasia following subcutaneous administration of the compound (HSDB, 1990). The liver damage reported in rabbits included fatty infiltration, and kidneys evidenced minute petechiae, larger ecchymises, or even lobular hemorrhage, depending on the degree of exposure (HSDB, 1990).

NB was fetotoxic when administered subcutaneously to pregnant rats during preimplantation and placentation. Delay of embryogenesis, alteration of normal placentation, and fetus abnormalities were observed (HSDB, 1990). However, no treatment-related effects were reported during organogenesis, indicating that there are no developmental, including teratogenic, effects following exposure to atmospheric levels up to 40 ppm for 6 hours/day on days 6 through 15 of gestation (HSDB, 1990).

EPA has classified NB as a group D (not classifiable) carcinogen, which indicates that there is inadequate or no evidence regarding the carcinogenicity of this compound. EPA has not addressed the carcinogenicity of DNB and TNB (IRIS, 1990; HEAST, 1990).

No evidence of mutagenicity was observed following exposure of Salmonella typhimurium strains to NB (HSDB, 1990).

3.1.3.2 Ecotoxicity

Aquatic Organisms

Acute toxicity to freshwater aquatic life occurs at concentrations of NB ranging from as low as 640 µg/L for the leopard frog to as high as 163,000 µg/L for the fathead minnow (see Table 3.1-9). In the alga Selenastrum capricomutum, 96-hour EC50 values of 42,800 and 44,100 µg/L were reported for reduced cell numbers and inhibition of chlorophyll a, respectively (EPA, 1980). Acute EC50 values for the cladoceran Daphnia magna range from 24,000 to 62,000 µg/L, and acute EC50 values for the bluegill range from 43,000 to 135,000 µg/L (EPA, 1980).

In chronic studies, concentrations as high as 32,000 µg/L produced no effects on fathead minnow embryos or larvae; however, no definitive chronic toxicity data are available (EPA, 1980).

Studies by Lu and Metcalf (1975) on green filamentous algae (Oedogonium cardiacium), snails (Physa spp.), Daphnia, mosquito larvae (Culex quinquifasciatus), and mosquitofish (Gambusia affinis) show that NB was neither stored nor biomagnified. NB was reduced to aniline in all organisms,

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Table 3.1-9. Acute Toxicity Values of NB to Aquatic Organisms

Scientific Name **(Common Name)**	Toxicity Value (µg/L)	Reference
Selenastrum capricomutum (Alga)	ECSO: 42,800 to 44,000	EPA, 1980e
Daphnia magna (Water Flea)	LC50: 24,000 to 27:000 EC50: 60,000	Leblanc, 1980 Kuhn et al., 1989*
Leuciscus idus (Golden orfe)	LC50: 50,000	Wellens, 1982
Pimephales promelas (Fathead minnow)	LC50: 117,000 to 163,000 LC50: 119,000	Holcombe et al., 1984 Geiger et al., 1985*
Oryzias latipes (High-eyes)	LC50: 20,000 to 24,000	Tonogai et al., 1982
Lepomis macrochirus (Bluegill)	LC50: 43,000 to 135,000	Buccafusco et al., 1981
Rana pipiens (Leopard frog)	LC50: 640 to >1,270	Black et. al., 1982

*From HSDB, 1990.

Source: Primary citations may not have been reviewed. Citations were derived from Aquatic Information Retrieval (AQUIRE), 1990.

from 16 to 24 days, depending on the presence of other compounds; in distilled water, the estimated half-life was reported to be 23 days, and the observed value was 69 days (LLNL, 1987). No hydrolysis is reported to occur for DNB (EPA, 1979; LLNL, 1987). DNB was oxidized in the laboratory by a 2-step process involving activated sewage sludge in conjunction with a microorganism (LLNL, 1987).

Volatilization is not expected to be an important migration pathway for DNB because of the low vapor pressure, which is reported as 1.31×10^{-4} mmHg at 25°C (LLNL, 1987; EPA, 1979).

3.1.4.1 Health Effects Assessment

EPA has derived an oral chronic and an interim oral subchronic RfD for DNB of 0.0001 mg/kg/day (IRIS, 1990) and 0.001 mg/kg/day (HEAST, 1990), respectively. The DNB oral RfD was derived from a study in which rats were provided drinking water containing either 3, 8, or 20 mg/L DNB; these doses are equivalent to 0.40, 1.1, and 2.7 mg/kg/day (IRIS, 1990). Increased spleen weights were observed at 8 mg/L, and decreased weight gain and hemoglobin concentrations, testicular atrophy, splenic enlargement, and hemosiderin deposits were reported at the high dose of 20 mg/L. Thus, for oral exposure, 0.4 mg/kg/day was set as the NOEL from which the chronic and subchronic RfDs are derived, and 1.1 mg/kg/day was set as the LOAEL. EPA has not derived any inhalation RfD values for DNB.

The principal toxic effects reported for DNB are the same as for NB because the primary responses to exposure are methemoglobinemia and liver dysfunction (HSDB, 1990). Following chronic exposure, symptoms included headache;

burning pain; and paresthesia in feet, ankles, hands, and the forearms. Apathy, shortness of breath, and heart palpitations were also reported. In addition, chronic exposure led to vision impairment, with visual fields slightly contracted; visual acuity, particularly for reds and greens, was reduced by central scotomas (HSDB, 1990). Although partial ocular atrophy occurs, vision does gradually recover (HSDB, 1990).

Symptoms reported for rats exposed to a l-percent suspension of DNB in corn oil included ataxia, dyspnea, rapid heartbeat, cyanosis, coma, and respiratory failure (HSDB, 1990). In a reproductive study, splenic hemosiderosis was reported in weanlings dosed as low as 0.75 mg/kg/day (HSDB, 1990). No additional experimental animal toxicity data were reported in the reviewed databases (IRIS, 1990; HEAST, 1990; HSDB, 1990).

Data indicate that DNB is a potent testicular toxicant in the male rat (HSDB, 1990). Decreased sperm production, decreased caudal epididymal sperm reserves, nonmotile spermatozoa, atypical sperm morphology, decreased weights of the testes and epididymides, seminiferous tubular atrophy, and incomplete spermatogenesis were all observed in male rats dosed at 3 mg/kg/day; sperm production was decreased in males dosed with 1.5 mg/kg/day (HSDB, 1990).

DNB was be mutagenic to Salmonella tyhimurium strains without metabolic activation (HSDB, 1990).

3.1.4.2 Ecotoxicity

Aquatic Organisms

In acute tests with freshwater organisms, bluegill and rainbow trout were the most sensitive vertebrate species to DNB, with 96-hour LC50 values of 1.44 and 1.70 mg/L, respectively (see Table 3.1-11). Van der Schalie (1983) performed a dynamic acute test with rainbow trout that lasted 30 days and produced an LC50 of 0.37 mg/L.

Only one species (rainbow trout) was found in a 68-day chronic test for DNB which produced results greater than the acute test for the same species by the same author (see Table 3.1-12). The greatest sensitivity for early life stage-no-effect concentration (ELS-NEC) was 0.44 mg/L (>0.37 mg/L in the acute test).

Terrestrial Organisms

See Sec. 3.1.4.2 for additional information on this compound as regards plants. No data were found on the effect(s) to terrestrial plants or animals other than those data noted in Sec. 3.1.3.1.

3.1.4.3 Criteria and Standards

See Sec. 3.1.4.2.

3.1.5 TNB

TNB is an explosive and, although it is less sensitive to impact than TNT, it is considered more powerful and brisant. No photolysis of TNB was reported (LLNL, 1987), nor was hydrolysis reported to occur for TNB (EPA, 1979; LLNL, 1987). TNB was oxidized in the laboratory by a 2-step process involving activated sewage sludge in conjunction with a microorganism (LLNL, 1987).

C-AAAPSRIFS.7/BEA-V.33
04/03/91

Table 3.1-11. Acute Toxicity of DNB to Aquatic Organisms

Scientific Name (Common Name)	Effect	S/F	Duration (hours or days)	Concentration hg/L)	Reference
INVERTEBRATES					
Daphnia magna	LC5O	S	48 hr	49.6	Liu et al., 1983 (LLNL, 1987)
	LC5O	S	48 hr	27.4	van der Schalie, 1983 (LLNL, 1987)
VERTEBRATES					
Oncorhvncus mykiss (was Salmo gairdneri) Rainbow trout)	LC5O	S	96 hr	1.70	van der Schalie, 1983 (LLNL, 1987)
	LC5O	F	30 days	0.37	van der Schalie, 1983 (LLNL l987)
Pimephales promelas (Fathead minnow)	LC5O	S	96 hr	7.0	Liu et al., 1983a (LLNL, 1987)
	LC5O	S	96 hr	7	Bailey and Spanggord, 1983 (LLNL, 1987)
	LC5O	S	96 hr	16.8	van der Schalie, 1983 (LLNL, 1987)
Lepomis macrochirus (Bluegill)	LC5O	S	96 hr	1.44	van der Schalie, 1983 (LLNL. 1987)
Ictalurus punctatus (Channel catfish)	LC5O	S	96 hr	8.13	van der Schalie, 1989 (LLNL, 1987)

Note: References in parentheses are secondary sources.

Source: ESE.

Table 3.1-12. Chronic Toxicity of DNB to Aquatic Organisms

Scientitic Name (Common Name)	Effect	S/F	Duration (hours or days)	Concentration (mg/L)	Reference
VERTEBRATES					
Oncorhyncus mykiss (was Salmo gairdneri) (Rainbow trout)	ELS-NEC	S	**68-day**	**0.84**	van der Schalie, 1983
	ELS-NEC	S	**68-day**	**0.97**	van der Schalie, 1983
	ELS-NEC	S	68-day	0.44*	van der Schalie, 1983
	ELS-NEC	S	68-day	0.50*	van der Schalie, 1983
	NEC			0.16*	van der Schalie, 1983

Note: S = static test.

*Because of the 96 hour flow-through, LC50 (see Table 3.1-11) is lower than the ELS-NEC. Using a value of 0.16 m/L as the NEC is recommended.

Source: LLNL, 1987.

Volatilization is not expected to be an important migration pathway for TNB because of the low vapor pressure, which is reported to be 3.03 x 10^{-6} mmHg at 25°C (LLNL, 1987; EPA, 1979).

3.1.5.1 Health Effects Assessment

Data on the toxicity of TNB are insufficient for deriving a RfD. Based on the rat oral LD50 values for DNB and TNB, which are 83 mg/kg-bw and 450 mg/kg-bw respectively, EPA deems it appropriate to use the DNB rat drinking water study to derive the RfD for TNB. Adjusting the 0.4 mg/kg/day for DNB for molecular weight difference, the corresponding equivalent intake was calculated to be 0.51 mg/kg/day (BUS, 1990). Because the RfD is derived by analogy to a structurally similar compound, a greater uncertainty factor was applied. The oral chronic and interim oral subchronic RfD values are 0.00005 mg/kg/day (IRIS, 1990) and 0.0005 mg/kg/day (HFAST, 1990), respectively.

The toxic effects reported for TNB are the same as for NB and DNB, consisting primarily of damage to the CNS and liver (HSDB, 1990). Death from any of these compounds, although uncommon, is usually due to cardiovascular collapse, and not respiratory paralysis (HSDB, 1990).

No data were presented regarding any reproductive effects of TNB (IRIS, 1990; HEAST, 1990; HSDB, 1990). TNB is mutagenic with several of the Salmonella typhimurium strains; however, metabolic activation reduced the magnitude of the responses (HSDB, 1990).

3.1.5.2 Ecotoxicity

Aquatic Organisms

Only one example was found in the literature regarding the acute effects of TNB to aquatic macrophytes (see Table 3.1-13). In tests using the algae Selenastrum capricomutum, van der Schalie (1983) reported a growth inhibition (with respect to controls) at all concentrations tested (ranging from 0.10 to 17.32 mg/L.)

In 48-hour acute tests with the water flea (Daphina magna), Liu et al. (1983a) reported an LC50 of 2.7 mg/L, and van der Schalie (1983) reported an EC50 at 2.98 mg/L (for immobilization). In completion of the 96-hour LC50 tests with fathead minnows, Bailey and Spanggord (1983) and Liu et al. (1983a) reported concentrations of 1.1 mg/L. However, tests by van der Schalie (1983) present conflicting data with results of 0.49 mg/L and 1.03 mg/L for the same species. Channel catfish was the most sensitive species at 0.38 rng/L (van der Schalie, 1983).

A 21-day chronic toxicity study with daphnia indicated that the no-effect range was between 0.47 and 0.75 mg/L, showing that these ‘invertebrates were less sensitive to TNB than the fathead minnow and rainbow trout (see Table 3.1-14).

Terrestrial Organisms

For data on the effects of 1,3,5-TNB to terrestrial organisms, see Sec. 3.1.3.1. No data were found regarding the effects of this compound to wildlife.

Table 3.1-13. Acute Toxicity of TNB to Aquatic Organisms (Continued, Page 2 of 2)

Species	Effect	S/F	Duration (hours)	Concentration (mg/L	Reference
Pimephales Promeles (Fathead minnow)	LC50	S	96		l.l Liu et al., 1983a (LLN, l987)
					O.Svan der Schalie, 1983 (LLNL, 1987)
	LC50	S	96		1.03van der Schalie, 1983 (LLNL, 1987)
	LC50	S	96		l.lBailey and Spanggord, 1983 (LLNL, 1987)
Lepomis macrochirus (Bluegill)	LC50	S	96		0.85van der Schalie, 1983 (LLNL, 1987)
Ictalurus punctatus (Channel catfish)	LC50	S	96		0.38van der Schalie, 1983 (LLNL, 1987)

Note: References in parentheses are secondary sources.

Source: ESE.

Table 3.1-14. Chronic Toxicity of TNB to Aquatic Organisms

Species	Effect	S/F	Duration (hours or days)	Concentration mg/L)	Reference
INVERTEBRATES					
Daphnia magna	NEC	S	21 days	0.47 to 0.75	van der Schalie, 1983
VERTEBRATES					
Oncorhyncus mykiss (Rainbow trout)	LC50	S	18 days	0.43	van der Schalie, 1983
pimenhales promeles (Fathead minnow)	LC50	S	10 days	0.46	van der Schalie, 1983
	ELS-LEC	S		0.12	van der Schalie, 1983
	ELS-NEC	S		0.08	van der Schalie, 1983

Note: ELS-LEC = early life stage-lowest-effect concentration.

Source: LLNL, 1987.

3.1.5.3 Criteria and Standards

No federal AWQC are available for TNB.

3.1.6 ANILINE

Aniline, which is toxic to humans, is a colorless to brown, oily liquid. Aniline and its methylated derivatives are used in the production of dyes, rubber, pesticides, and pharmaceuticals and in the oil and coal industry.

3.1.6.1 Chemical and Physical Properties

Property	Value	References
Chemical formula	$C_6H_5NH_2$	Joseph, 1985
Molecular weight	93.14	Sax and Lewis, 1989
Boiling point	184°C	Joseph, 1985
Melting point	6.2C	Joseph, 1985
Water solubility	3.5	Joseph, 1985
Vapor pressure	0.6 mmHg	Joseph, 1985
Henrys law constant	1.2×10^{-4}	HSDB, 1990
K_{oc}	NA	NA
$Log_{10} K_{ow}$	NA	NA
Kd	NA	NA

Note: NA = not available.

3.1.6.2 Fate and Transport

Aniline and its derivatives are found in industrial wastewater effluents and in soils mainly as a degradation product of herbicides. In water, aniline decomposes by microbial degradation and photooxidation. Adsorption to sediments and humic materials is moderate and occurs predominantly under

acidic conditions; sorption to colloids is high and may accelerate leaching in groundwater (HSDB, 1990). In air, aniline is photodegradable (HSDB, 1990).

3.1.6.3 Health Effects Assessment

EPA has not derived either oral or inhalation RfD values for aniline (IRIS, 1990; HEAST, 1990). Although methemoglobin is the most prominent noncarcinogenic symptom of aniline toxicity in humans, acute toxicity also causes CNS symptoms, including dyspnea; tachycardia; headache; dizziness; and, in severe cases, possible photophobia, weakness of vision, and slow pupillary action (HSDB, 1990). Other symptoms include cardiac effects, such as heart blocks, arrhythmia, and shock; fatalities usually occur because of cardiovascular collapse and respiratory paralysis (HSDB, 1990).

Acute animal toxicity studies have found that, for most species, the oral LD50 ranges from 440 mg/kg-bw to 500 mg/kg-bw; a similar range of values is reported for dermal exposure (Berkowitz et al., 1978). Acute exposure to aniline leads to the formation of methemoglobin (Doull et al., 1986), which is followed by a corresponding depression of the CNS. The exposure of rabbits to doses up to 50 mg/kg-bw resulted in cyanosis and coma, but no methemoglobin was reported (Berkowitz et al., 1978). Rats exposed to a dose of 22 mg/day in drinking water for a lifetime evidenced SO-percent mortality by day 450 and 100 percent mortality by day 750 (IRIS, 1990). Following the exposure of rats, mice, guinea pigs, and dogs to 5 ppm concentrations in air, only rats evidenced an increase in methemoglobinemia (HSDB, 1990).

EPA (IRIS, 1990) has classified aniline as a group 82 (probable human) carcinogen for oral and inhalation exposure. This classification indicates that

data are insufficient regarding the carcinogenicity in humans but that sufficient animal carcinogenicity data exist. The oral cancer slop factor is 0.0057 $(mg/kg/day)^{-1}$; no inhalation value is available. The primary animal data were derived from a study in which rats were exposed to aniline hydrochloride at dietary levels of 200, 600, or 2,000 mg/kg-feed for 2 years (IRIS, 1990). Splenic sarcomas were observed in the high-dose males, and lesions considered to be precursors to the sarcomas were observed in the high-dose males and, to a lesser degree, in the female rats. Following exposure to aniline hydrochloride at dietary levels of either 3,000 or 6,000 mg/kg-feed for 2 years, statistically significant increases in hemangiosarcomas and fibrosarcomas were observed in the high-dose male rats; other sarcomas were also observed to be increased in the high-dose males (IRIS, 1990). Mice provided food containing aniline hydrochloride at either 6,000 or 12,000 mg/kg evidenced no carcinogenic effects (IRIS, 1990). Rats provided drinking water containing up to 0.12-percent aniline either alone or in combination with the co-mutagen norhaman for 80 weeks evidenced no carcinogenic effects (IRK, 1990).

Aniline was generally nonmutagenic to Salmonella typhimurium except in the presence of the co-mutagen norharman (HSDB, 1990). It was mutagenic in a lymphoma gene mutation assay and caused increased sister chromatid exchanges in vivo in mice and chromosomal aberrations (HSDB, 1990). It was identified as a potential developmental toxin in mammals and amphibians (HSDB, 1990).

3.1.6.4 Ecotoxicity

Aquatic Organisms

Baxrerton et al. (1978) conducted algal assays and liquid culture toxicity tests on several species of blue-green algae, other algae, and bacteria. Results showed that blue-green algae are much more sensitive to aniline and p-toluidine, a methylated derivative, than are the other organisms.

In a study by Witherspoon (1980), population density of Chlorella vulgaris fluctuated with corresponding fluctuations in aniline concentrations in a dye-manufacturing plant waste effluent. In a study a Chlorella (Amman and Terry, 1985), aniline concentrations of 183.9 ppm affected growth, respiration, and photosynthesis. Primary production would be affected over time through sublethal exposures and could be eliminated altogether (Amman and Terry, 1985).

In acute LC50 tests, Daphnia were the most sensitive species tested; midge, snails, and goldfish were the most resistant (see Table 3.1-15). In studies on amphibians, acute LC50 values ranged from 440 to 560 mg/L (HSDB, 1990). Information on chronic studies was not found in the available literature.

Aniline does not bioaccumulate in fish, although it is absorbed and metabolized (HSDB, 1990). For three fish species, the log BCFs are 0.78, 1.0, and 5, and for algae, the log BCF is 0.60 (HSDB, 1990). Aniline is a metabolite of NB, and bioaccumulation via this pathway may occur as well (EPA, 1980).

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Table 3.1-15. Acute LC50 Values of Aniline in Selected Aquatic Species

Scientific Name	*Common Name* or Group	LC50 value	Water Hardness *(mg/L* $CaCO_3$	Reference*
Tanytarsus dissimilis	Midge	>219	NA	Holcombe et al., 1987
Apexa hypnorum	Snail	>210	NA	Holcombe et al., 1987
Daphnia pulex, D. cucculata, and D. magna	Water Flea	0.1 to 0.68	NA	Canton, 1978; Bringham and Kuehn, 1977; Holcombe et al., 1987
Ambystoma mexicanum	Mexican axolotl	440	NA	Verscheuren, 1983
Xenopus laevis	Clawed toad	560	NA	Sloof and Baersecman, 1980
Micropterus sp.	Bass	5.2 to 47.3 4.4 to 43.2	so 200	Marking and Kimerle, 1979 Marking and KimerIe, 1979
Lepomis macrochitus	Bluegill	49.0	NA	Holcombe et al., 1987
Carascius auratus	Goldfish	5.5 to 10.2 4.7 to 10.0 187	50 200 NA	Marking and Kimerle, 1979 Marking and Kimerle, 1979 Holcombe et al., 1987
Ictalurus punctatus	Catfish	5.6 5.0 to 7.4	50 200	Marking and Kimerle, 1979 Marking and Kimerle, 1979
Leuciscus idus melanotus	Golden orfe	51 to 92	NA	Juhnke, 1978
Oncorhyncus mykiss	Rainbow trout	8.2 to 40.5	NA	Abram and Sims, 1982; Holcombe et al., 1987
Pimephales promelas	Fathead minnow	77.9 134	NA 47	Holcombe et al., 1987 Brooke et al., 1984
Catostomus commersoni	White sucker	78.4	NA	Holcombe et al., 1987

Note: NA = not available.

*References cited from HSDB, 1990.

Source: ESE.

Terrestrial Organisms

In studies conducted on the effects of aniline on seedling crops, Nozzolillo (1971) reported that germination and pigmentation were affected and abnormal development occurred following a dose of 0.01 to 0.05 M aniline; root tip destruction was a major deformity. Growth was completely inhibited in bush beans and runner beans at concentrations of 0.03 to 0.05 M.

Results of vertebrate studies report an oral LD50 for rats of 250 mg/kg, an inhalation LC_{LO} of 250 ppm per 7 hours, and an LD50 of 1,400 mg/kg (Sax and Lewis, 1989). At dietary levels of 10, 30, or 100 mg/kg, changes in spleen function were noted (HSDB, 1990). The oral LD50 for dogs is 195 mg/kg, and the skin LD_{LO} is 1,540 mg/kg (Sax and Lewis, 1989). In rabbits, oral and skin LD_{LO} values are 1,000 mg/kg and 820 mg/kg, respectively.

No information was found in the available literature for chronic study results or BCF data.

3.1.6.5 Criteria and Standards

The OSHA permissible exposure limit (PEL) for humans reports skin exposure of S ppm [time-weighted average (TWA)]; the ACGIH TLV reports 2 ppm (TWA) (Sax and Lewis, 1989). No AWQC are available for aniline.

3.2 ASBESTOS

Asbestos is a generic term applied to numerous naturally occurring, fibrous mineral silicates. Asbestos minerals are separated into two major groups, serpentine (which includes the mineral chrysotile) and amphibole (which includes the minerals amosite, crocidolite, anthophyllite, tremolite, as well as

actinolite minerals). Chrysotile is the major type of asbestos used in the manufacture of asbestos products such as asbestos cement pipe, flooring products, paper products (e.g., padding), friction materials (e.g., brake linings and clutch facings), rooting products, and coating and patching compounds (EPA, 1980a).

3.2.1 HEALTH EFFECTS ASSESSMENT

Asbestos risks are limited to workplace exposure only.

3.2.2 ECOTOXICITY

3.2.2.1 Aquatic Organisms

Few data exist currently concerning the effects of asbestos on freshwater aquatic organisms. In fish tissue studies analyzed by transmission electron microscopy, however, microscopic inorganic particles of asbestos were found. Tissue samples obtained from organisms in a river with known chrysotile asbestos contamination and brook trout, lake trout, and channel catfish exposed to water contaminated with amphibole fibers contained mineral fibers identical to those in the water. Muscle tissue concentrations were about one-twelfth the average water concentrations by volume, but liver and kidney fiber concentrations were 500 times greater than muscle tissue concentrations (HSDB, 1990).

Mussels (Mytilus edulis) exposed to water containing asbestos mine tailings in concentrations up to 100 mg/L were examined after exposure. Fibers were found in the epithelial tissue of the stomach and intestinal tract and persisted *even* when the mussels were kept in unpolluted water for several weeks.

Appendix F4
Aster Ecotoxicity Profiles

U.S. Environmental Protection Agency
Environmental Research Laboratory-Duluth

Contact: Scientific Outreach Program
218-720-5602 or fax 218-720-5539

Rep 118-96-7 2,4,6-Trinitrotoluene

I. CHEMICAL IDENTIFICATION

Name	2,4,6-Trinitrotoluene
CAS number	118-96-7
SMILES	c(c(cc1N(=O)=O)N(=O)=O)c(c1C)N(=O)=O
Formula	C7 H5 N3 06

II. ENVIRONMENTAL EXPOSURE ASSESSMENT

Parameter	Value	Source	Reference
Molecular Weight (g/mole)	227.1	Calc.	
Melting Point (C)	82.0	ASTER	
Boiling Point (C)	391	Calc.	
Vapor Pressure (mm of Hg)	1.49E-08	talc.	
Ht Vaporization (Cal/mole)	1.84E+04	talc.	
Solubility in Water (mg/L)	7.16E+03	talc.	
Log P	1.46	CLogP	3573
pKa	not available for this chemical		
Adsorption Coef (log Koc)	2.13	talc.	
Henry's Constant (atm-m**3/mole)	6.20E-13	talc.	

Parameter	Value	Source	Reference
Henry's Constant (atm-m**3/mole)	6.20E-13	Calc.	
Log10 (Henry's Constant) (atm-m**3/mole)	-12.2	Calc.	
Hydrolysis Half-life (days)	hydrolysis unlikely		
BOD Half-life:	HALF LIFE 2 TO 16 DAYS	Calc.	

Mackay Level 1 Environmental Partitioning @25 C Fugacity = 8.938E-13 Pa

0.00 % into air
0.23 % into soil
99.56 % into water
0.00 % into suspended solids
0.00 % into aquatic biota
0.21 % into sediment

III. ECOTOXICOLOGICAL HAZARD ASSESSMENT

Aquatic Hazard Identification

ACUTE DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
20482: scud Hyalella azteca	S	2.00	LC50	MOR		6500	AQUIRE	6502
20481: Water flea Daphnia magna	S	2.00	LC50	MOR		11900	AQUIRE	6502

BIOCONCENTRATION DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
128007: Fathead minnow Pimephales promelas	F	2.00-304	BCF	RSD	calcu-lated	6	QSAR	7

OTHER DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
20480: Oligochaete Lumbriculus variegatus	s2	2.00	LC50	MOR		4900	AQUIRE	6502
20483: Midge Tanytarsus dissimilis	S	2.00	LC50	MOR		24800	AQUIRE	6502

Human Health Hazard Identification

There is no information in the QSAR SYSTEM which would suggest that this chemical is a potential carcinogen or mutagen.

IV. ECOLOGICAL RISK CHARACTERIZATION

A. Environmental Exposure Assessment

Henry's Constant = 6.20E-13 atm-m**3/mole
Log10 (Henry's Constant) = -12.2 atm-m**3/mole

Lyman et al. 1982 would conclude that a chemical with these properties is non-volatile. See page 15-15.

Hydrolysis is not likely to be an important transformation mechanism for this chemical.

B. Ecotoxicological Hazard Assessment

Genetic/Mutagenic Assessment

There is no information in the QSAR SYSTEM which would suggest that this chemical is a potential carcinogen or mutagen.

REACTIVE DINITRO GROUP Dinitroaromatic compounds have generally been associated with an intoxication syndrome that is consistent with a chemical reactivity-based mode of action. This reactivity may be the result of two electron metabolic reductions to electrophilic nitroso compounds [178] or one electron reductions to nitro anion free radicals that redox cycle with oxygen, resulting in oxidative stress [3410].

When sufficient data is available from fathead minnow early life stage (ELS) tests (32-d exposures) completed at ERL-Duluth, QSAR models have been developed to predict chronic values for either survival or growth, which ever is the most sensitive endpoint. A chronic value is defined as the geometric mean of the LOEC (lowest observable effect concentration) and the NOEC (no observable effect concentration). These models have been developed for groups of xenobiotics that have been classified based on their acute modes of toxic action. Empirical observations suggest that when a statistically robust ELS QSAR can be established and when 96-h LC50/32-d ELS chronic value ratios are within a factor of 20 it is reasonable to assume that adverse effects are elicited through the same mode of toxic action in both 4-d and 32-d exposures. If during a chronic exposure a different mode of action is involved, or if metabolic activation is significant, the ratios between acute and chronic endpoint values for a group of xenobiotics are generally quite variable and typically exceed two orders of magnitude. In addition, the statistical strength of ELS QSARs in these instances are poor.

A chronic value cannot be calculated for the fathead minnow for chemicals with a reactive mode of action. 96-h LC50/32-d ELS chronic value ratios for reactive toxicants tested at ERL-Duluth using the fathead minnow range from 1 to 19.5 (log P range of 0.21 to 7.54).

C. Other Information

More information on this chemical is available through the US EPA's Office of Health and Environmental Assessment's IRIS (Integrated Risk Information System) data base.

V. CITATION INFORMATION

REFERENCE NUMBER: 7

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1983

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In: D. Mackay et al., (Eds.), Physical Behavior of PCBs in the Great Lakes, Ann Arbor Science Publishers, Ann Arbor, MI:269-282

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Deneer, J.W., T.L. Sinnige, W. Seinen, and J.L.M. Hermens

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Quantitative Structure-Activity Relationships for the Toxicity and Bioconcentration Factor of Nitrobenzene Derivatives towards the Guppy . . .

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Environ. Health Perspect. 87:237-243

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Information Systems, Inc., 3951 Claremont St., Irvine, C.A. 92714

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Bailey, H.C. and D.H.W. Liu

1980

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In: J.C. Eaton, P.R. Parrish, and A.C. Hendricks (Eds.),

Aquatic Toxicology and Hazard Assessment, 3rd Symposium,

ASTM STP 707, Philadelphia, PA:205-215

OTHER DATA FROM AQUIRE

ASTER processes all Ecotoxicological Hazard Assessment information through a filter which removes data from the final Report which may not be of the highest quality. This appendix contains Other Data that did not meet the filter requirements, but is contained in the AQUIRE database.

ACUTE DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
31278: Water flea Daphnia magna	S	2.00	EC50	IMM		11900		5087
40133: Water flea Daphnia magna	S	2.00	LC50	MOR		6600		6021
63020: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2200		6041
63021: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2100		6041
63022: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2200		6041
63023: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2700		6041
63024: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2800		6041

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
63025: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		4100		6041
63026: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2700		6041
63027: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		2800		6041
63028: Bluegill Lepomis macrochirus	R	4.00	LC50	MOR		2300		6041
63029: Bluegill Lepomis macrochirus	R	4.00	LC50	MOR		1600		6041
63030: Bluegill Lepomis macrochirus	R	4.00	LC50	MOR		2300		6041
63031: Bluegill Lepomis macrochirus	R	4.00	LC50	MOR		2300		6041
20477: Bluegill Lepomis macrochirus	S	4.00	LC50	MOR		3000		6502
33459: Fathead minnow Pimephales promelas	F	4.00	LC50	MOR		2580		926
122680: Fathead minnow Pimephales promelas	F	4.00	LC50	MOR		1600		926
122680: Fathead minnow Pimephales promelas	S	4.00	LC50	MOR		2400		5087
40132: Fathead minnow Pimephales promelas	S	4.00	LC50	MOR		2400		6021
40135: Fathead minnow Pimephales promelas	S	4.00	LC50	MOR		1200		6021
40137: Fathead minnow Pimephales promelas	S	4.00	LC50	MOR		2000		6021
20484: Fathead minnow Pimephales promelas	S	4.00	LC50	MOR		3100		6502
71225: Fathead minnow Piiephales promelas	S	4.00	LC50	MOR		3000		10141

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
20479: Channel catfish Ictalurus punctatus	S	4.00	LC50	MOR		2400		6502
20478: Rainbow trout, donaldson trout Oncorhynchus mykiss	S	4.00	LC50	MOR		1200		6502

PLANT DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
36218: Green algae Selenastrum capricomutum	S	7.00		PGR		2500		2476
36218: Green algae Selenastrum capricomutum	S	7.00		PGR		1000		2476
46514: Duckweed Lemna perpusilla	S	11.0		PGR		1000		8706
46515: Duckweed Lemna perpusilla	S	11.0		PGR		500		8706
46516: Duckweed Lemna perpusilla	S	11.0		PGR		100		8706
46517: Duckweed Lemna perpusilla	S	11.0		PGR		1000		8706
MEDIA NOT REPORTED								
37241: Green algae Scenedesmus quadricauda	S	NR		MOR		1600		2463
20988: Green algae Scenedesmus qluadricauda	S	NR		PGR		1600		7453

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
24994: **Green algae** **Scenedesmus quadricauda**	**S**	**7.00**		**PGR**		**1600**		**5303**
57370: Green algae Scenedesmus quadricauda	S	8.00		PGR		1600		15134
33461: Green algae Scenedesmus quadricauda	S	13.0		PGR		7000		926
16758: Cryptomonad Chilomonas paramecium	NR	2.00		PGR		5400		5719
24995: Flagellate euglenoid Entosiphon sulcatum	S	3.00		PGR		1600		5303
37240: Blue-green algae Anacystis aeruginosa	S	NR		MOR		320		2463
57371: Blue-green algae Anacystis aeruginosa	S	8.00		PGR		320		15134
33463: Blue-green algae Anacystis aeruginosa	S	17.0		PGR		50000		926
28080: Blue-green algae Anacystis aeruginosa	S	1.00	LETH	MOR		8000		8065

OTHER DATA

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
FRESHWATER								
87879: Water flea Daphnia magna	S	1.00	EC0			9mg/L		707
114398: Water flea Daphnia magna	S	1.00	EC100			23mg/L		707

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
94441: Water flea Daphnia magna	S	1.00	EC50			18 mg/L		707
20989: Water flea Daphnia magna	S	1.00	LC50	MOR		14000		5718
33460: Fathead minnow Pimephales promelas	F	4.00	EC50	BEH		460		926
122681: Fathead minnow Pimephales promelas	F	4.00	EC50	BEH		460		926
40134: Fathead minnow Pimephales promelas	S	1.00	LC50	MOR		4200		6021
40136: Fathead minnow Pimephales promelas	S	1.00	LC50	MOR		>3200		6021
40138: Fathead minnow Pimephales promelas	S	1.00	LC50	MOR		3000		6021
115906: Rotifer Brachonus calyciflorus	S	2.00	EC50	REP		4000		3963
115907: Rotifer Brachionus calyciflorus	S	2.00	LC50	MOR		9100		3963
115905: Rotifer Brachionus calyciflorus	S	2.00	LOEC	REP		5000		3963
115904: Rotifer Brachionus calyciflorus	S	2.00	NOEC	REP		2300		3963
SALTWATER								
36220: Harpacticoid copepod Tigriopus califomicus	S	3.00		MOR		2500		2476
36221: Harpacticoid copepod Tigriopus califomicus	S	3.00		MOR		1000		2476

Species Common Name Species Latin Name	Ex Ty	Dur (days)	End point	Effect	Conc Type	Conc (ug/L)	Source	Ref No.
36222: **Pacific oyster** **Crassostrea gigas**	**S**	**4.00**		**MOR**		**5000**		**2476**
36223: Pacific oyster Crassostrea gigas	S	4.00		MOR		10000		2476

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